Benactyzine

Other names:	Benzeneacetic acid, «alpha»-hydroxy-«alpha»-phenyl-, 2-(diethylamino)ethyl ester
	Benzilic acid, 2-(diethylamino)ethyl ester
	Benactyzin
	Benactizina
	Benzilic acid «beta»-diethylaminoethyl ester
	Diazil
	Diethylaminoethyl benzilate
	«beta»-Diethylaminoethyl benzilate
	2-(Diethylamino)ethyl benzilate
	2-(Diethylamino)ethyl diphenylglycolate
	Diphenylglycolic acid 2-(diethylamino)ethyl ester
	«alpha»-Hydroxy-«alpha»-phenylbenzeneacetic acid 2-(diethylamino)ethyl ester
	2-Diethylaminoethyl benizilate
	Diethyl(2-hydroxyethyl)amine benzilate
	Benactizine
Inchi:	InChI=1S/C20H25NO3/c1-3-21(4-2)15-16-24-19(22)20(23,17-11-7-5-8-12-17)18-13-9-6-1
InchiKey:	IVQOFBKHQCTVQV-UHFFFAOYSA-N
Formula:	C20H25NO3
SMILES:	CCN(CC)CCOC(=O)C(O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	327.42
CAS:	302-40-9

Physical Properties

Property code	Value	Unit	Source
gf	85.22	kJ/mol	Joback Method
hf	-321.32	kJ/mol	Joback Method
hfus	38.12	kJ/mol	Joback Method
hvap	91.25	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.808		Crippen Method
mcvol	268.430	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2249.00		NIST Webbook
rinpol	2249.00		NIST Webbook
rinpol	2248.00		NIST Webbook
rinpol	2230.00		NIST Webbook

rinpol	2248.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2248.00		NIST Webbook
tb	888.04	K	Joback Method
tc	1105.29	K	Joback Method
tf	535.87	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.21	J/mol×K	888.04	Joback Method
cpg	854.04	J/mol×K	924.25	Joback Method
cpg	866.85	J/mol×K	960.46	Joback Method
cpg	878.73	J/mol×K	996.67	Joback Method
cpg	889.79	J/mol×K	1032.88	Joback Method
cpg	900.12	J/mol×K	1069.08	Joback Method
cpg	909.80	J/mol×K	1105.29	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C302409&Units=SI

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume